CHARGE NUMBER: 2520

PROJECT TITLE: Synthesis of Flavorants

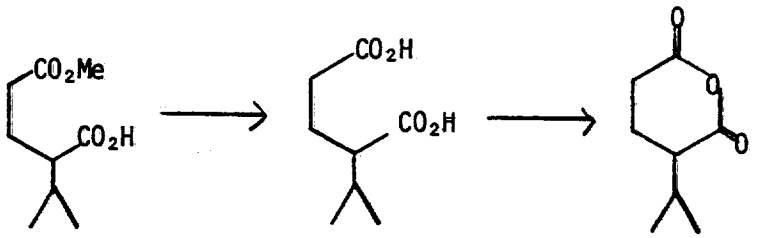
PROJECT LEADER: William B. Edwards, III

PERIOD COVERED: August 1-31, 1981

DATE OF REPORT: September 9, 1981

I. Terpenoid Flavorants[1]

Saponification of 4-carbomethoxy-2-isopropylbutanoic acid (I) gave the tobacco identical 2-isopropylpentanedioic acid (II). The acid (II) has a cheesy, valeric acid odor. Purification of II by gas chromatography is not possible, as the diacid dehydrates to the anhydride (III) under GC conditions. A sample of III will be prepared for flavor evaluation.



I II III

A mixture of methyl cis-4-isopropyl-7-methyl-5,7-octadienoate (IV, 20%) and methyl trans-4-isopropyl-7-methyl-5,7-octadienoate (V, 80%) was prepared from methyl 4-isopropyl-5-oxopentanoate via Wittig reaction with methallylidenetriphenylphosphorane. Following separation of the isomers, V will be hydrolyzed to the tobacco identical acid.

IV V

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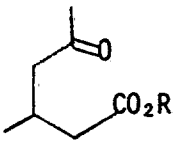
With the purification of the esters (VIa-d) and the synthesis/ purification of the ester (VIe), our work for a patent disclosure on long chain esters of oxoacids is completed.



R= a) $-CH_2(CH_2)_8CH_3$

b) $-CH(CH_2)_5CH_3$
$CH_2CH_2CH_3$

c) $-CHCH_3$
$CH_2(CH_2)_{12}CH_3$

d) $-CH_2(CH_2)_{20}CH_3$

e) $-CH_2(CH_2)_7CH=CH(CH_2)_7CH_3$

1) D. Williams: N.B. 7618

William A. Williams

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